THE LASER RAMAN SPECTRA OF LARGE DIAMONDOID MOLECULES: A ROUTE TO UNDERSTANDING NANODIAMOND CRYSTALS

P.W. May, J. Filik, J.N. Harvey

School of Chemistry, University of Bristol, Bristol BS8 1TS, U.K.

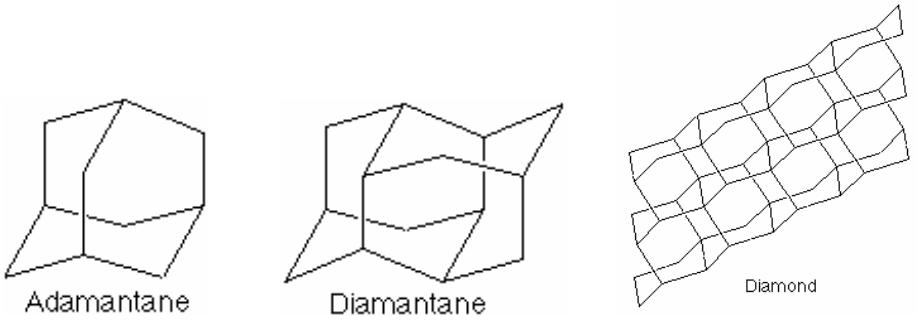
J.E.P. Dahl, R.M.K. Carlson and S. Liu

MolecularDiamond Technologies, ChevronTexaco Energy Technology Co.,
P.O. Box 1627, Richmond, CA 94802, USA.

Keywords: Diamondoids, nanodiamond, adamantane, laser raman spectroscopy

Abstract

Diamond is composed of tetrahedrally-bonded carbon atoms, and the simplest molecule with the diamond structure is adamantane ($C_{10}H_{16}$). Diamondoids of the adamantane series are hydrocarbons composed of fused cyclohexane rings, all in stable chair conformations, which form interlocking cage structures that can be superimposed on the diamond crystal lattice. The lower diamondoids have chemical formulas of $C_{4n+6}H_{4n+12}$, where n equals the number of diamond-cage subunits.



Diamondoids occur naturally in virtually all petroleum, and have been extracted by reverse phase high performance liquid chromatography (HPLC), and then isolated and recrystallised by standard organic chemistry techniques. A whole series of these diamondoid crystals from $n = 1$ (adamantane) to 10 (decamantane) have been studied by laser Raman spectroscopy using 3 laser wavelengths (325, 514 and 735 nm). The spectra have also been simulated using theoretical predictions using the Gaussian program, and this has allowed the experimental peaks to be assigned to individual vibrational motions. The larger diamondoids are similar in size to the nanodiamond grains grown during CVD of ultra-nanocrystalline diamond (UNCD) films, and so the Raman spectra of these diamondoids provides insights into the interpretation of spectra from UNCD films.